computers & chemistry

An International Journal

Editor: David Edelson

List of Contents and Author Index
Volume 15, 1991

PERGAMON PRESS
Oxford New York Seoul Tokyo

computers & chemistry

An International Journal

editor

David Edelson: Department of Chemical Engineering, FAMU/FSU College of Engineering, P.O. Box 2175, Tallahassee, FL 32316-2175, U.S.A.

consulting editor

DeLos F. DeTar: Department of Chemistry, Florida State University, Tallahassee, FL 32306-3006, U.S.A.

editorial board

Dr A. M. Bond
Department of Chemistry
La Trobe University
Bundoora, Vic. 3083
AUSTRALIA

Josef Brandt
Institut für Organische Chemie
Technische Universität München
Lichtenbergstrasse 4
8046 Garching
FED. REP. GERMANY

Dr J. Crabbe
Department of Microbiology
University of Reading
Reading RG1 5AQ
ENGLAND

Dr Istvan Csorvassy
Alkaloida, 4440 Tiszavasvari
HUNGARY

Dr Johann Gasteiger
Organische-Chemisches Institut
Technische Universität München
8046 Garching
FED. REP. GERMANY

Professor Peter A. Kollman
Department of Pharmaceutical Chemistry
University of California
San Francisco, CA 94143
U.S.A.

Professor George Levy
Department of Chemistry
Syracuse University
Syracuse, NY 13210
U.S.A.

Professor James A. McCammon
Department of Chemistry
University of Houston
Houston, TX 77004
U.S.A.

Dr Carl Moser
CECAM
Université de Paris XI
91405 Orsay
FRANCE

Professor Iwao Ohmine
Institute for Molecular Science
Myodaiji-Machi
Okazaki-shi 444
JAPAN

Dr Arthur Olson
Research Institute of the Scripps Clinic
10666 North Torrey Pines Road
La Jolla, CA 92037
U.S.A.

Professor Eiji Osawa
Department of Knowledge-based Info Engineering
Toyohashi University of Technology
Tempaku-cho, Toyohashi 440
JAPAN

Dr Shin-ichi Sasaki
Toyohashi University of Technology
Tempaku-cho
Toyohashi 440
JAPAN

Professor Isaiah Shavitt
Department of Chemistry
Ohio State University
Columbus, OH 43210
U.S.A.

Professor Nenad Trinajstic
Institut Rugjer Boskovic
P.O. Box 1016
41001 Zagreb
Croatia
YUGOSLAVIA

Professor Dr Ivar Ugi
Organisch-Chemisches Institut
Technische Universität München
8046 Garching
FED. REP. GERMANY

Dr Bastiaan van de Graaf
University of Technology
Juliana Laan 136
2528 BL Delft
THE NETHERLANDS

Professor Charles L. Wilkins
Department of Chemistry
University of California
Riverside, CA 92521
U.S.A.

Liaison Members:
Professor Guido Buzzi-Ferraris
(Computers & Chemical Engineering)
Dipartimento di Chimica Industriale e Ingegneria Chimica Politecnico di Milano
Piazza Leonardo da Vinci 32
20133 Milano
ITALY

Dr Luis C. Puigjaner
(Computers & Chemical Engineering)
Universidad Politecnica de Cataluna
Escuela Tecnica Superior de Ingenieros Industriales de Barcelona
Departmento de Ingenieria Química
Catedra de Technologia
Química General
Diagonal 647, 08028 Barcelona
SPAIN

Professor Ervin Y. Rodin *(Computers & Mathematics with Applications)*
Department of Systems Science and Mathematics
Washington University
Box 1040, St Louis, MO 63130
U.S.A.

Publishing Office: Pergamon Press plc, Pergamon House, Bampfylde Street, Exeter EX1 2AH, England [*Tel.* (0392) 51558; *Fax* 425370].

Subscription and Advertising Offices: *North America*—Pergamon Press Inc., 395 Saw Mill River Road, Elmsford, NY 10523, U.S.A.; *Rest of the World*—Pergamon Press plc, Headington Hill Hall, Oxford OX3 0BW, England [*Tel.* (0865) 794141; *Fax* 60285].

Subscription Rates: annual institutional subscription rate (1992): £245.00 (US$390.00); 2-year institutional rate (1992/93): £465.50 (US$741.00). Sterling prices are definitive. U.S. dollar prices are quoted for convenience only, and are subject to exchange rate fluctuation. Prices include postage and insurance and are subject to change without notice. Subscription rates for Japan are available on request.

Back Issues: back issues of all previously published volumes, in both hard copy and on microform, are available direct from Pergamon Press offices.

Published Quarterly. Copyright © 1991 Pergamon Press plc

It is a condition of publication that manuscripts submitted to this journal have not been published and will not be simultaneously submitted or published elsewhere. By submitting a manuscript, the authors agreee that the copyright for their article is transferred to the publisher if and when the article is accepted for publication. However, assignment of copyright is not required from authors who work for organizations which do not permit such assignment. The copyright covers the exclusive rights to reproduce and distribute the article, including reprints, photographic reproductions, microform or any other reproductions of similar nature and translations. No part of this publication may be reproduced, stored in a retrieval system or transmitted in any form or by any means, electronic, electrostatic, magnetic tape, mechanical, photocopying, recording or otherwise without permission in writing from the copyright holder. Whilst every effort is made by the publishers and editorial board to see that no inaccurate or misleading data, opinion or statement appears in this journal, they wish to make it clear that the data and opinions appearing in the articles and advertisements herein are the sole responsibility of the contributor or advertiser concerned. Accordingly, the publishers, the editorial board and editors and their respective employees, officers and agents accept no responsibility or liability whatsoever for the consequences of any such inaccurate or misleading data, opinion or statement.

Photocopying information for users in the U.S.A. The Item-fee Code for this publication indicates that authorization to photocopy items for internal or personal use is granted by the copyright holder for libraries and other users registered with the Copyright Clearance Center (CCC) Transactional Reporting Service provided the stated fee for copying, beyond that permitted by Section 107 or 108 of the United States Copyright Law, is paid. The appropriate remittance of $3.00 per copy per article is paid directly to the Copyright Clearance Center Inc., 27 Congress Street, Salem, MA 01970, U.S.A.

Permission for other use. The copyright owner's consent does not extend to copying for general distribution, for promotion, for creating new works, or for resale. Specific written permission must be obtained from the publisher for such copying.

The Item-fee Code for this publication is: 0097-8485/91 $3.00 + 0.00

♾™The text paper used in this publication meets the minimum requirements of American National Standard for Information Sciences—Permanence of Paper for Printed Library Materials, ANSI Z39.48-1984.

List of Contents

NUMBER 1

Wolfgang Linert, Peter Margl and **Ernst Nusterer**	1	The use of enhanced operator–machine interfaces in computer aided molecular design
S. Lalitha, G. V. R. Chandramouli and **P. T. Manoharan**	11	Calculation of charges from photoelectron spectra
C. Muller, G. Scacchi and **G. M. Côme**	17	A topological method for determining the external symmetry number of molecules
Miguel A. Raso, J. Tortajada and **F. Acción**	29	A general fitting program for resolution of complex profiles—II. Automatic baseline correction
Michael L. Connolly	37	Molecular interstitial skeleton
Jan K. Labanowski, Ioan Motoc and **Richard A. Dammkoehler**	47	The physical meaning of topological indices
M. V. Mirkin and **A. P. Nilov**	55	Modification of the Huber method for solving integral equations on a non-uniform grid
J. F. Ogilvie	59	General linear regression analysis—application to the electric dipole-moment function of HCl
Manfred J. Sippl and **Hans Stegbuchner**	73	Superposition of three-dimensional objects: a fast and numerically stable algorithm for the calculation of the matrix of optimal rotation
Michael J. Mitchell and **J. Andrew McCammon**	79	Vector optimization of AMBER 3.0 on the NEC SX-2/400 supercomputer
Software Notes		
M. T. Oms, R. Forteza, V. Cerdà, F. García-Sánchez and **A. L. Ramos**	87	FLUOROPACK: a program package for automatic fluorimetric measurements
Gy. Dömötör and **M. I. Bán**	91	Program for orientating crystal surfaces
Peter Senn	93	Determination of the position of an atom in space from three interatomic distances

Book Review
Peter Lykos 95 Expert System Applications in Chemistry: ACS Symposium Series 408, edited by B. A. Hohne and T. H. Pierce

NUMBER 2

Ü. Haldna, M. Grebenkova and **A. Ebber** 99 A new approach to the analysis of the UV absorption spectra of ketones in aqueous sulfuric acid

Alf Dengler and **Ivar Ugi** 103 A central atom based algorithm and computer program for substructure search

Janusz Gawłowski, Krzysztof Franaszczuk, Mirosław Jaśkiewicz and **Jan Niedzielski** 109 Modernization of the MX-1321 mass-spectrometer: a new information system for GC/MS analysis

W. S. Verwoerd and **V. Nolting** 115 An improved molecular orbital localization scheme

Jeroen van Westrenen, Peter L. Khizhnyak and **Gregory R. Choppin** 121 Speciation of complexes by Lotus 1–2–3

J. M. Lisý, A. Cholvadová and **B. Drobná** 127 Least squares analysis—propagation of random errors and Newton–Raphson iterative formula

J. M. Lisý, A. Cholvadová and **B. Drobná** 135 Polynomial (linear in parameters) least squares analysis when all experimental data are subject to random errors

János Lejtovicz 143 A computer program for the deficiency zero and deficiency one theorems

C. L. do Lago and **C. Kascheres** 149 New method of isotope pattern analysis

Kenneth J. Tupper, Richard W. Counts and **Joseph J. Gajewski** 157 Geometry optimization within a modified Extended Hückel formalism: modifications to the ASED program

Horst Lueck, Maurice W. Windsor and **Ralf Menzel** 161 Fully-automated excited state measurements with enhanced dynamic range by interfacing a Quantel laser YG501 and an optical multichannel analyzer PAR 1205B to an IBM PC/XT

Michael V. Mirkin 169 Computer modeling 3-D nucleation and growth

Software Note
R. Fausto and **J. J. C. Teixeira-Dias** 175 NBI: a FORTRAN program for molecular mechanics calculations on a microcomputer

I Announcements

NUMBER 3

Alicia Batana, Celia Finazzi de Andrade and **Inés Gomez**	179	Grüneisen parameters of a hexagonal close-packed lattice
Roy T. Ing	185	MOLLY—a language for typesetting molecular structure diagrams
Shridhar R. Gadre, Sangeeta Bapat and **Indira Shrivastava**	203	Computation of molecular electrostatic potential: an efficient algorithm and parallelization
B. Fourest, F. David, E. Haltier, N. Borome, A. Richard, D. Lecouturier and **G. Lalu**	207	A rapid scanning spectrophotometer: applications to some spectroelectrochemical experiments
S. C. Lee and **Soo-Y. Lee**	215	A rapid method for determining excited state surface parameters and bond length in diatomic molecules and calculating wavefunctions for Franck–Condon factors using the quantum momentum method
A. Batana and **J. A. O. Bruno**	225	Calculation of the effective charge of crystals and its volume dependence
Software Note		
José Miguel Rodríguez Mellado	235	A convolution algorithm for linear-sweep voltammetric data at unequally spaced times
Book Reviews		
Terry W. Clark	237	Methods in Computational Chemistry, Vol. 3: Concurrent Computations in Chemical Calculations, edited by Stephen Wilson
DeLos F. DeTar	238	PCs for Chemists, edited by J. Zupan
Jerzy Cioslowski	238	Large Order Perturbation Theory and Summation Methods in Quantum Mechanics, by G. A. Arteca, F. M. Fernández and E. A. Castro

A Selection of Papers Presented
at
THE SECOND BIENNIAL WORKSHOP ON MOLECULAR MECHANICS AND MOLECULAR DYNAMICS

DeLos F. DeTar	v	Introduction
Minoru Hirota, Kazuhisa Sakakibara, Tamiki Komatsuzaki and **Ikuo Akai**	241	A new steric substituent constant Ωs based on molecular mechanics calculations
K. Palmö, L.-O. Pietilä and **S. Krimm**	249	Conversion of *ab-initio* force fields and structures to molecular mechanics energy functions

Tamar Schlick 251 New approaches to potential energy minimization and molecular dynamics algorithms

M. Geller, A. Łączkowski, S. M. Swanson and **E. F. Meyer Jr** 261 Dynamical analysis of the conformation of the active site of porcine pancreatic elastase in native and Michaelis complex states. Molecular dynamics simulations

Laurence Leherte, Jean-Marie Andre, Eric G. Derouane and **Daniel P. Vercauteren** 273 Study of the water behavior into a ferrierite zeolite by molecular dynamics simulations

J. D. Pulfer 287 Numerical modelling of the action of acetolactate synthase isozyme II using simplex optimization

NUMBER 4

Luca Baumer, Giordano Sala and **Guido Sello** 293 Ring perception in organic structures: a new algorithm for finding SSSR

F. Humbert, A. Retournard, J. Brondeau and **D. Canet** 301 Fast bidirectional NMR data transfer between the Bruker Aspect 3000 and a personal computer

L. A. Berrueta, L. A. Fernandez and **F. Vicente** 307 FLUORIM: a computer program for the automated data collection and treatment using commercial spectrofluorimeters

Xiang Xiong, Yu-Zhen Zhu and **Xin Zhou** 313 A simple microcomputer-controlled instrumental system for kinetic analyses and determinations

S. Bhattacharjee, A. S. Rao and **P. Dasgupta** 319 A new index for molecular property correlation in halomethanes

J. M. Figuera, J. Luque, V. Menendez and **J. C. Rodriguez** 323 An algorithm for the determination of the vibrational energy distribution in "hot" molecules. Description and test

W. F. Cooper and **W. L. Parker** 333 An inexpensive personal computer based photon counter

C. Muller, G. Scacchi and **G. M. Côme** 337 A compiler for a linear chemical notation

Software Notes

Peter Senn 343 Accurate and efficient computation of Γ-functions with complex arguments

Hanna Mazurkiewicz-Łazowska and **Piotr Paneth** 347 Numerical evaluation of the time-dependence of concentrations, rates and kinetic isotope effects